# COMPSCI 688: Probabilistic Graphical Models

## Lecture 13: Introduction to Markov Chain Monte Carlo

Dan Sheldon

Manning College of Information and Computer Sciences
University of Massachusetts Amherst

Partially based on materials by Benjamin M. Marlin (marlin@cs.umass.edu) and Justin Domke (domke@cs.umass.edu)





# A Quiz Question





## A Quiz Question

Consider an exponential family on $x_1, x_2 \in \{0,1\}$ with $T(x_1, x_2) = \mathbb{I}[x_1 = 1, x_2 = 1]$.
Suppose you use the data below to estimate maximum likelihood parameters:

| $x_1$ | $x_2$ |
|---|---|
| 1 | 1 |
| 1 | 0 |
| 1 | 1 |
| 0 | 1 |

At the maximum likelihood estimate $\theta^*$, what will be $P_{\theta^*}(X_1 = 1, X_2 = 1)$?

# Application Example





## Covid Model

Showed Covid modeling example w/ NumPyro. See Jupyter notebook





# Monte Carlo Methods





## Motivation

Computing expectations is important!

$$\mathbb{E}_{p(x)}[f(X)] = \int p(x)f(x)dx$$

**Example**: suppose $p(\mathbf{x})$ is an MRF, then

$$P(X_u = a, X_v = b) = \mathbb{E}_{p(\mathbf{x})}\left[\mathbb{I}[X_u = a, X_v = b]\right]$$

In general, computing expectations is hard, so we need an approximation.

## Monte Carlo methods

In a Monte Carlo method, we approximate an expected value by a sample average. Draw $N$ samples $X_1, \dots, X_N \sim p(x)$, then

$$\mathbb{E}_{p(x)}[f(X)] \approx \frac{1}{N} \sum_{n=1}^{N} f(X_n).$$

Nice properties:

- Unbiased
- Variance decreases like $\frac{1}{N}$.
- Measure arbitrary properties by choosing $f$.

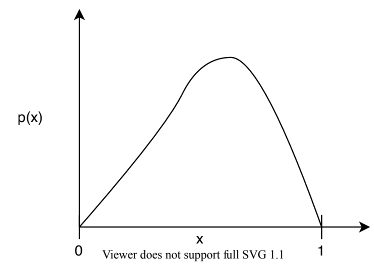
Not nice properties: **sampling is algorithmically/computationally hard** in general





## Examples

Suppose we have $p(x) = 12(x^2 - x^3)$, where $x \in [0, 1]$. Or suppose we have an MRF with a cycle.




**Question**: How do we sample from these distributions? Answer: We need an algorithm.





## Gibbs Sampling





## Markov Chain Monte Carlo Overview

- Markov chain Monte Carlo (MCMC) methods *iteratively* construct samples from a given “target distribution” $p(\mathbf{x})$
- They require only access to the *unnormalized* distribution, so can apply easily to models like MRFs.
- Formally, they work by constructing a *Markov chain* that has the target distribution $p(\mathbf{x})$ as its limiting distribution.
- We’ll introduce one MCMC method today, and then start to develop some of the theory needed to understand the algorithm.
- Importance / applications: statistical physics, econometrics, ecology, epidemiology, weather modeling, ...

## The Gibbs Sampler

A simple and powerful algorithm! Assume $\mathbf{X} = (X_1, \dots, X_D)$.

Initialize all variables arbitrarily, then repeatedly update each variable by sampling from its conditional distribution given all other variables.

**Gibbs sampler**

- Initialize $x_1, \dots, x_D$
- Repeat
  - For $i = 1$ to $D$, resample $x_i \sim p(X_i \,|\, \mathbf{X}_{-i} = \mathbf{x}_{-i})$
  - Record $\mathbf{x} = (x_1, \dots, x_D)$ as one sample

One sample is generated after each loop through all of the variables.





## Example: Cycle MRF

Suppose $p(\mathbf{x}) = \prod_{i=1}^{n} \phi(x_i, x_{i+1})$ (mod $n$)

Then $p(x_i|\mathbf{x}_{-i}) \propto \phi(x_{i-1}, x_i)\phi(x_i, x_{i+1})$ (factor reduction!)

For a general MRF: $p(x_i|\mathbf{x}_{-i}) \propto \prod_{c:i \in c} \phi_c(x_i, \mathbf{x}_{c \setminus i})$





## The Gibbs Sampler: Properties

- The Gibbs sampler eventually draws samples from the target distribution $p(\mathbf{x})$ regardless of how it is initialized.
- It can take time to converge to the target distribution $p(\mathbf{x})$. This phase of the algorithm is referred to as the “burn-in” phase of the algorithm.
- Convergence to the target distribution needs to be tested empirically in most cases using convergence diagnostics.
- Even after convergence, the samples **are not independent**, but can still be used in Monte Carlo averages. The degree of correlation of the samples affects the rate of convergence of Monte Carlo averages.